Numerical Optimization

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Team

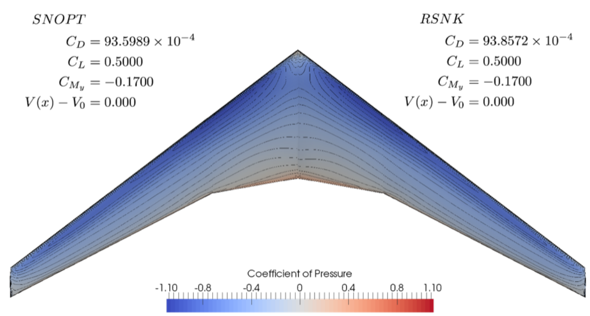
- Alp Dener (ANL) – Large-scale optimization
- Xiang Huang (ANL) – Composite optimization
- Sven Leyffer (ANL) – Discrete optimization
- Juliane Müller (LBNL) – Sensitivity analysis
- Todd Munson (ANL) – Large-scale optimization
- Mauro Perego (SNL) – Inverse problems
- Ryan Vogt (NCSU) – Discrete optimization
- Stefan Wild (ANL) – Multi-objective optimization

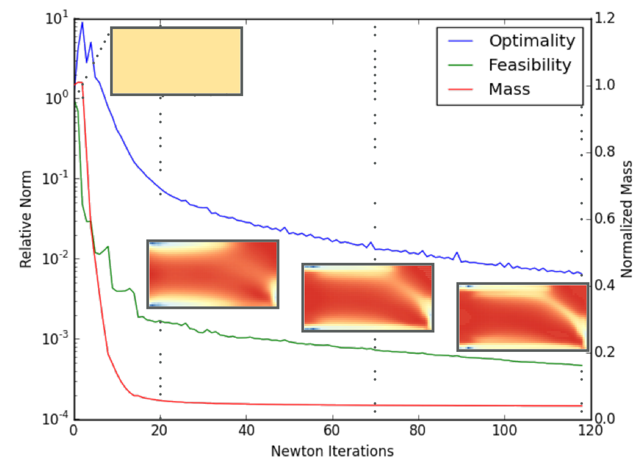
TAO Large-Scale Solvers: Preconditioned Nonlinear Conjugate Gradient

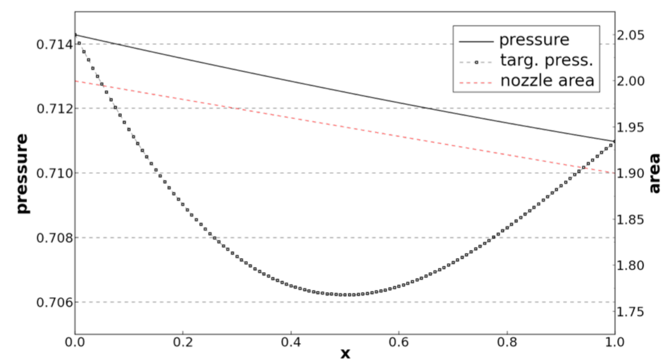
- **Problem formulation**

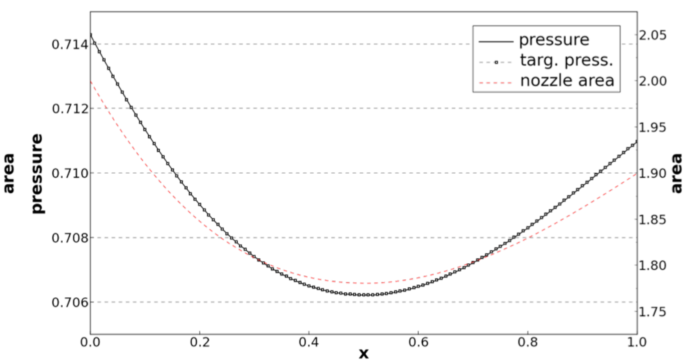
$$\min_{x} \quad f(x)$$
$$\text{s.t.} \quad b_l \le x \le b_u$$

- **Continuous and discrete**
- **Convex and nonconvex**
- **PDE-constrained**
  - **Engineering design**
  - **Data assimilation**
  - **Inverse problems**
  - **Design of experiments**
  - **Simulation-based control**
- **Data analysis**
  - **Sparse regression**
  - **Joint sparsity**









$$\underset{\mathbf{x}}{\text{minimize}} \quad f(\mathbf{x}) = \int_0^1 \frac{1}{2}\left(\mathbf{p}(\mathbf{x}) - \mathbf{p}_{\text{targ}}\right)^2 d\mathbf{x}$$

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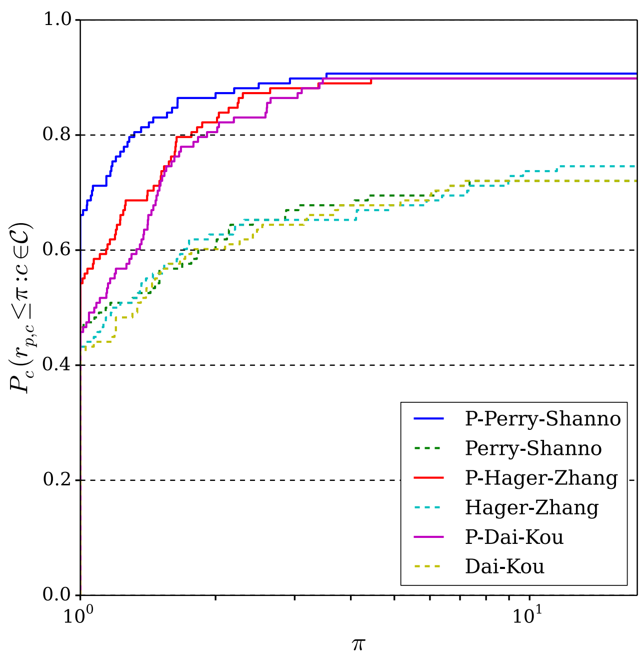
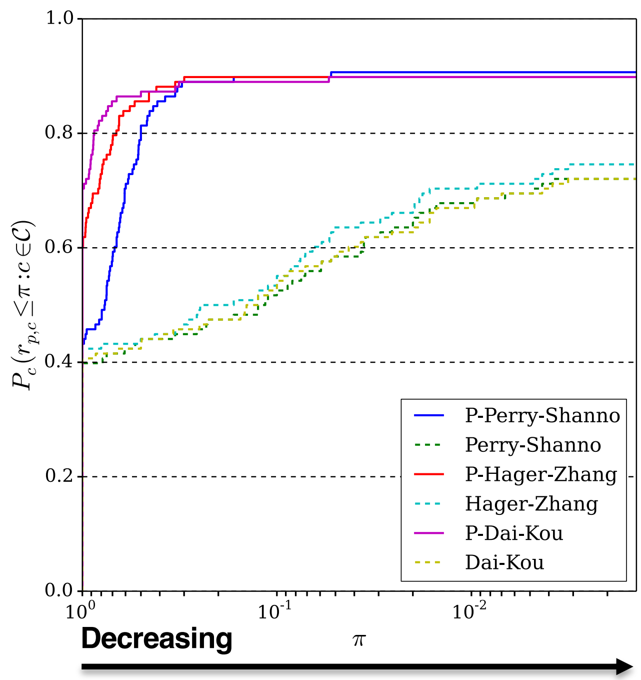
Alp Dener and Todd Munson (ANL), and Adam Denchfield (UIC)

TAO Large-Scale Solvers: Preconditioned Nonlinear Conjugate Gradient

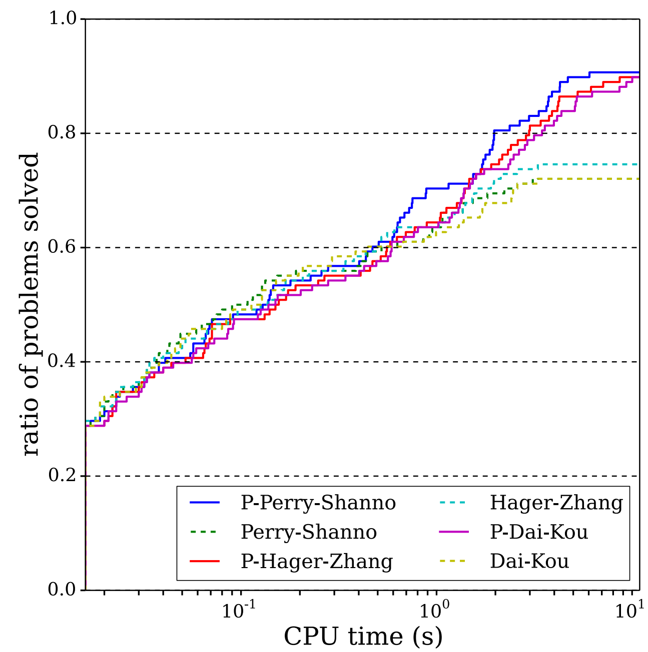
- **Preconditioned nonlinear conjugate gradient can be competitive with quasi-Newton with smaller memory footprint**
  - **Diagonalized quasi-Newton formula makes a good preconditioner for modern nonlinear conjugate gradient methods**
  - **Quasi-Newton-based preconditioner reduces reliance on specialized line searches**



(a) Comparison preconditioned to nominal methods based on function/gradient evaluations



(b) Comparison preconditioned to nominal methods based on linesearch steplength



(c) Comparison preconditioned to nominal methods based on time

Alp Dener and Todd Munson (ANL), and Adam Denchfield (UIC)

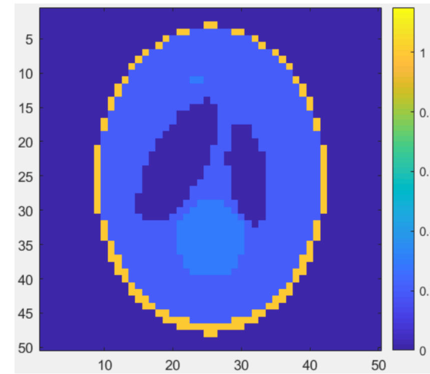
TAO Composite Optimization Solver for Sparse Regression

- **Developed a solver for composite optimization with a smooth term and a non-smooth joint-sparse regularizer term**

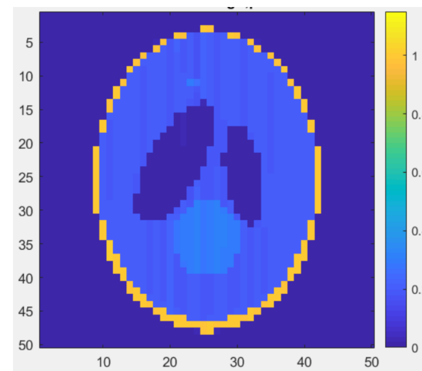
$$\min_{\mathbf{l} \leq \mathbf{x} \leq \mathbf{u}} \quad \frac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 + \tau\|\mathbf{D}\mathbf{x}\|_1,$$

where $\mathbf{A} \in \mathbb{R}^{M\times N}, \mathbf{x} \in \mathbb{R}^{N\times 1}, \mathbf{b} \in \mathbb{R}^{M\times 1}, \mathbf{D} \in \mathbb{R}^{K\times N}, \tau > 0$, and $\|\mathbf{x}\|_1 := \sum_{i=1}^{N} |\mathbf{x}_i|$.

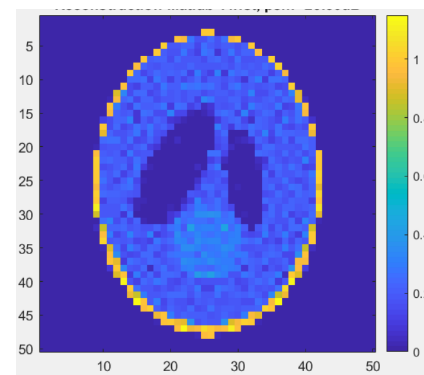
  - **Construct a smooth approximation and apply the Gauss-Newton method**
  - **Provides flexibility to include joint sparsity with a dictionary transform and bounds**
  - **Available in PETSc/TAO 3.11 release**
- **Solver is scalable and suitable for large-scale joint-sparse regression applications, such as tomography reconstruction**
- **Demonstrated superior performance compared to widely-used TwIST solver**



(a) Ground truth for comparison



(b) Our solver, PSNR = 46.01 dB



(c) TwIST solver, PSNR = 29.30 dB

Our method applied to tomography reconstruction. It shows that our solver yields 16.71 dB better when compared to the existing TwIST solver using similar computation time.

Xiang Huang, Alp Dener, and Todd Munson (ANL)

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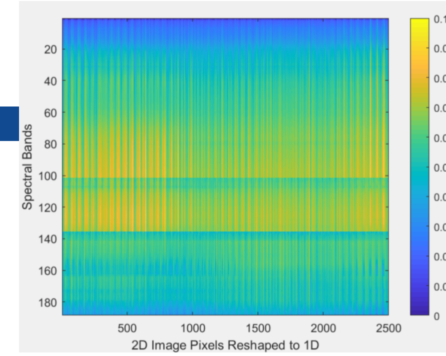
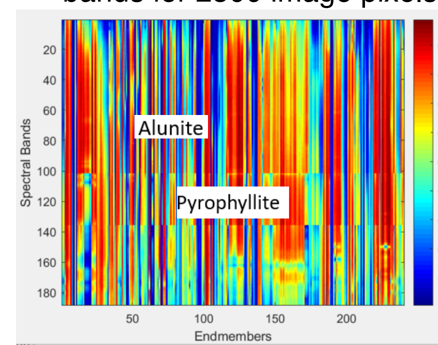
TAO Composite Optimization Solver with Joint-Sparsity Regularization



(a) Matrix B: 188 hyperspectral bands for 2500 image pixels



(b) Matrix A: 188 hyperspectral bands of 240 “minerals”

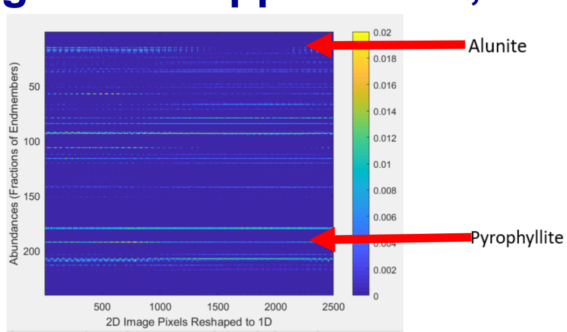
- **Developed a solver for composite optimization with a smooth term and a non-smooth joint-sparse regularizer term**

$$\min_{\mathbf{L} \leq \mathbf{X} \leq \mathbf{U}} \quad \frac{1}{2}\|\mathbf{AX}-\mathbf{B}\|_F^2 + \tau\|\mathbf{DX}\|_{2,1},$$

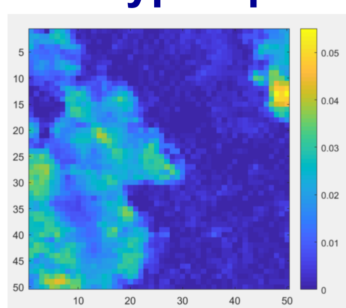
where $\mathbf{A} \in \mathbb{R}^{M\times N}, \mathbf{X} \in \mathbb{R}^{N\times L}, \mathbf{B} \in \mathbb{R}^{M\times L}, \mathbf{D} \in \mathbb{R}^{K\times N}, \tau > 0,$

$$\|\mathbf{X}\|_F^2 := \sum_{i=1}^N \sum_{j=1}^L \mathbf{X}_{ij}^2, \text{ and } \|\mathbf{X}\|_{2,1} := \sum_{i=1}^N \sqrt{\sum_{j=1}^L \mathbf{X}_{ij}^2}.$$

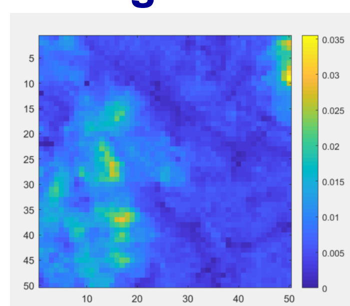
  - **Construct a smooth approximation and apply the Gauss-Newton method**
  - **Provides flexibility to include joint sparsity with a dictionary transform and bounds**
  - **Available in next PETSc/TAO release**
- **Solver is scalable and suitable for large-scale joint-sparse regression applications, such as hyperspectral image un-mixing**



(c) Computed X: fractions of 240 “minerals” for 2500 image pixels



(d) Alunite component



(e) Pyrophyllite component

Figure: Joint-sparsity reconstruction for hyperspectral un-mixing. (a) Cuprite sample, 188 spectral bands and 50x50 image pixels. (b) 240 pure spectral signatures. (c) Solution. (d) & (e) Alunite and Pyrophyllite reconstructions.

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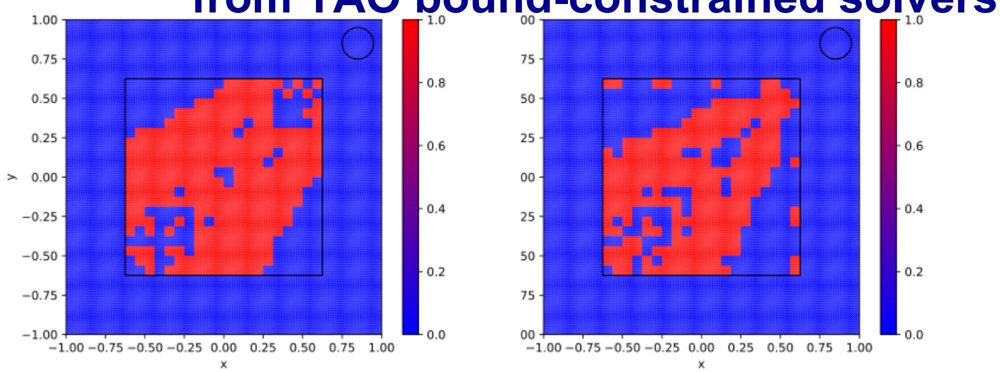
Discrete Optimization Methods
Design of an Electromagnetic Cloaking Device

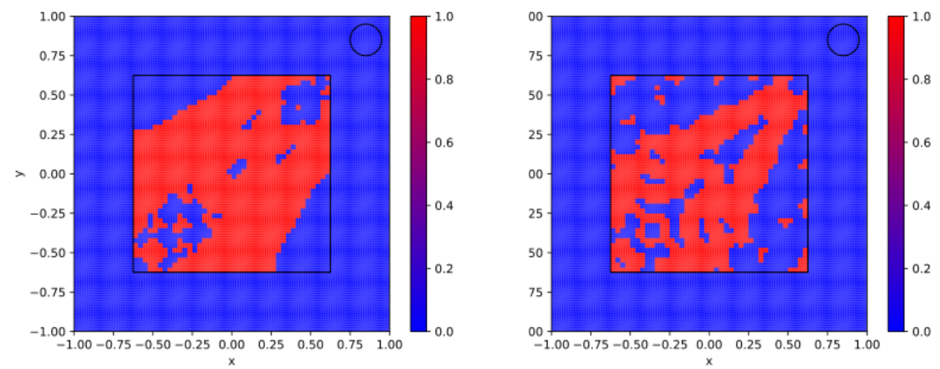
- **Developed a model for designing an electromagnetic cloaking device**

$$
\begin{aligned}
P(\theta) = \underset{v}{\text{minimize}} \quad & J(u) = \frac{1}{2}||u - u_0(\theta)||^2_{2,D_0} \\
\text{subject to} \quad & -\Delta u_{\text{Re}} - k_0^2(1+qw)u_{\text{Re}} = k_0^2 qw\cos(k_o(\cos(\theta)x + \sin(\theta)y)) && \text{in } D \\
& -\Delta u_{\text{Im}} - k_0^2(1+qw)u_{\text{Im}} = k_0^2 qw\sin(k_o(\cos(\theta)x + \sin(\theta)y)) && \text{in } D \\
& \frac{\partial u_{\text{Re}}}{\partial n} = -k_o u_{\text{Im}} \quad \text{and} \quad \frac{\partial u_{\text{Im}}}{\partial n} = k_o u_{\text{Re}} && \text{on } \partial D \\
& w = v_n && \text{in } \hat{\Omega}_n \ \forall n = 1, \ldots, N \\
& w = 0 && \text{in } D \setminus \left(\cup_n \hat{\Omega}_n\right) \\
& v_n = \{0, 1\} && \forall n = 1, \ldots, N.
\end{aligned}
$$

- **Produced robust model that considers multiple angles**
- **Developed trust-region method to refine relaxed, rounded solutions obtained from TAO bound-constrained solvers**



(a) Nominal and robust design for 20x20 control mesh



(b) Nominal and robust design for 20x20 control mesh

Sven Leyffer and Todd Munson (ANL) and Ryan Vogt (NCSU)

Application interactions

- *NP:* Nuclear Computational Low Energy Initiative (NUCLEI) – PI Joe Carlson (LANL), Stefan Wild
  - Calibration and optimization of energy density functionals
  - Support and modeling extensions for POUNDERS
  - Integration with UQ (w/ E. Lawrence, LANL)
- *HEP:* Community Project for Accelerator Science & Simulation (ComPASS4) – PI Jim Amundson (Fermilab), Stefan Wild
  - New optimization platform for particle accelerator design
  - Applications and extensions of POUNDERS
- *HEP:* Accelerating HEP Science: Inference and Machine Learning at Extreme Scales – PI Salman Habib (ANL), Juliane Müller & Stefan Wild
  - Development of methods for multi-fidelity optimization
  - Accelerate Bayesian parameter estimation with optimization (w/ R. Gramacy & D. Higdon, VTech)
  - Modeling and solvers for goal-oriented ML-based regression
- *HEP:* Data Analytics on HPC – PI Jim Kowalkowski (Fermilab), Sven Leyffer & Juliane Müller
  - Least-squares problems with integer variables and without derivatives
  - Sensitivity analysis integrated in optimization algorithms for expensive black-box problems
- *BER:* Probabilistic Sea-Level Projections from Ice Sheet and Earth System Models – PI Stephen Price (LANL), Juliane Müller & Mauro Perego
  - Optimization capability in Albany for solving transient large-scale PDE-constrained optimizations problems
  - Integrate efficient optimization methods in BISICLES initialization